

First-principles calculation of spin transport in magnetic nanowire using Green's function method with localized basis set

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Abstract. We report ab-initio calculations of the spin-dependent transport and magnetoresistance of Ni atom wires. The electronic states are calculated using a numerical pseudo atomic orbital basis set in the frame work of the density functional theory, and the conductance is calculated using the Green's function method. We show a magnetoresistance of 250%, which is explained by the scattering of d orbital channels.

1. Introduction

The investigation on spin-dependent transport phenomena is important not only for fundamental physics but also for applications in spin electronics, and much effort has been made for investigations on spin transport and magnetoresistance since the discovery of giant magnetoresistance.[1] Recent developments in experimental techniques have made it possible to fabricate nanoscale systems, and spin transport in nanostructures has also come to attract much attention.

The quantum effect is dominant in transport properties of nanostructures, and quantized conductance has been observed in atomic scale contacts and atomic wires. Regarding magnetic materials, spin-dependent quantized conductance and the enhancement of magnetoresistance have been observed.[2]-[5] Theoretically, the enhancement and oscillation of magnetoresistance have been shown for the constriction potential[6], and spin-dependent transport has been calculated for the atomic wire.[7]

We have developed a method of analyzing the quantum transport properties of nanoscale systems in the framework of density functional theory. We have applied the method to the analysis of the transport properties of a single molecule and carbon nanotubes between metallic electrodes.[8, 9] In this study, we analyze the spin-dependent transport and magnetoresistance in atomic wires using our method. We show the spin-dependent transmission spectra and

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magnetoresistance of nickel atom wire. We reveal that the magnetoresistance shows a value of 250% owing to the scattering of d orbital channels.

2. Method of Calculation

The system consists of atomic wire sandwiched between semi-infinite electrodes, and is divided into three regions. The Hamiltonian is partitioned as

$$H = \begin{pmatrix} H_L & H_{LC} & 0 \\ H_{CL} & H_C & H_{CR} \\ 0 & H_{RC} & H_R \end{pmatrix}. \quad (1)$$

The matrix elements of the Hamiltonian are obtained using calculations for a periodic system in the framework of the density functional theory with the local spin density approximation using a localized basis set of pseudo atomic orbitals.[10] As an atomic ion-core potential, a separable form of normconserving nonlocal pseudopotential[11, 12] is used. The retarded Green's function G_c is obtained as

$$G_c = [ES - H_c - \Sigma_L - \Sigma_R]^{-1}. \quad (2)$$

Here, the self energies Σ_L and Σ_R for the left and right electrodes are obtained using the Green's function of the semi-infinite electrodes.

The conductance G of the system is obtained from the Green's function using the Landauer formula and the Fisher-Lee relation[13]-[17] as

$$G = \frac{2e^2}{h} \text{Tr}[tt^\dagger], \quad (3)$$

$$= \frac{2e^2}{h} \text{Tr}[\Gamma_L G_c \Gamma_R G_c^\dagger]. \quad (4)$$

The coupling constant $\Gamma_{L(R)}$ is expressed as the imaginary part of the self-energies as

$$\Gamma_{L(R)} = i(\Sigma_{L(R)} - \Sigma_{L(R)}^\dagger). \quad (5)$$

The Hermitian matrix, tt^\dagger , formed from a product of the transmission matrices t is diagonalized using a unitary matrix U to transform the original channels into eigenchannels.

$$\text{Tr}(Utt^\dagger U^\dagger) = \sum \tau_n \quad (6)$$

The total conductance is expressed as a sum of the eigenchannel transmissions τ_n at the Fermi energy. In this basis, the scattering state in each channel is independent of each other without inter-channel scattering. [18, 19, 20]

3. Results and Discussions

We consider 6 Ni atoms in the conductor region between semi-infinite atomic wire electrodes. The interatomic distance is taken to be 2.1 Å. We use the pseudo atomic orbital basis set of Ni6.0-s2p2d2.

When the magnetizations of the electrodes are parallel, the transmission shows integer values corresponding to the number of bands of infinite atom wires formed by the $s - d_{z^2}$, d_{xz} , d_{yz} , d_{xy} , and $d_{x^2-y^2}$ orbitals as shown in Fig. 3. The z axis is taken to be parallel to the atomic wire. At the Fermi energy, all orbitals contribute to the transport for the up spin state, and only the $s - d_{z^2}$ orbital contributes to the transport for the down spin state. Therefore, the conductance is $7e^2/h$.

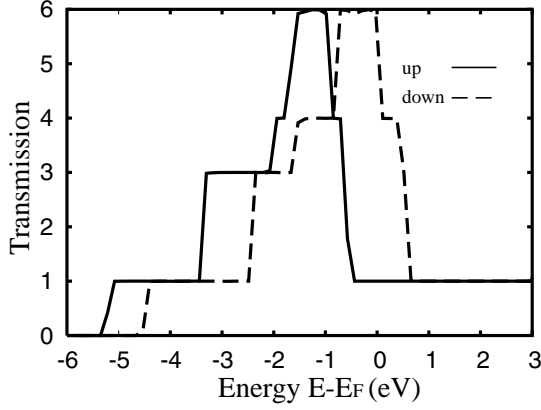


Figure 1. Transmission spectrum of Ni atom wire between parallel magnetizations of electrodes.

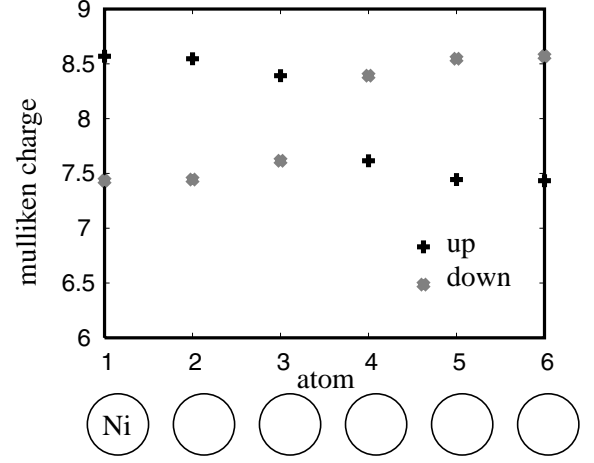


Figure 2. mulliken charges of Ni atom wire between antiparallel magnetizations of electrodes.

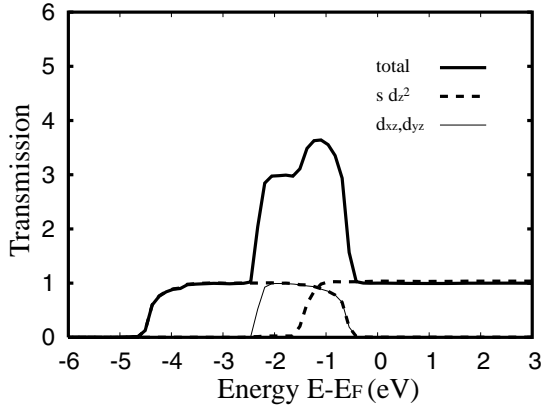


Figure 3. Total transmission and channel transmission spectra of Ni atom wire between antiparallel magnetizations of electrodes.

When the magnetizations of the electrodes are antiparallel, the domain wall is included in the conductor region as shown in Fig. 2, which depicts the mulliken charges for the spin states of the 4s, 3p and 3d orbitals at each atom. The change of the mulliken charges due to the domain wall is seen around only two atoms. Figure 3 shows the transmission spectrum for the antiparallel alignment. The transmission is the same for up and down states for the symmetry. In this case, the d states with a small momentum in the direction of atomic wires do not transport owing to the scattering at the domain wall, and only the $s - d_{z^2}$ states contribute to the transport. Thus, the conductance is $2e^2/h$, which corresponds to the plane-wave calculation.[7]

The magnetoresistance defined by $MR = (G_P/G_A) - 1$, where $G_{P(A)}$ is the conductance for the parallel (antiparallel) alignment of the electrode magnetization, is calculated to be 250%, which is consistent with the point contact experiment showing the magnetoresistance in excess of 200% [3]. The transport properties are sensitive to the geometries of the contact and the electrodes[20], and the small quantitative difference is expected to be due to the difference between the theoretical and experimental atomic configurations.

4. Summary

We analyzed the spin transport and magnetoresistance of a Ni atom wire using first-principles calculations. The electronic states were calculated using a numerical pseudo atomic orbital basis set in the framework of density functional theory, and the conductance was calculated using the Green's function method. The magnetoresistance of the wire was shown to be 250% owing to the scattering of d orbital channels.

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